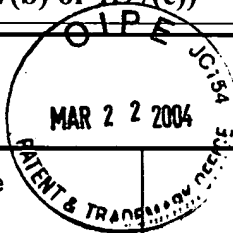


TRANSMITTAL OF INFORMATION DISCLOSURE STATEMENT
(Under 37 CFR 1.97(b) or 1.97(c))

Docket No.
30/1183US

In Re Application Of: **Randy J. Zauhar**



Serial No.
10/635,280

Filing Date
08/06/03

Examiner
TBD

Group Art Unit
TBD

Title: **Computer aided ligand-based and receptor-based drug utilizing molecular shape**

Address to:

**Assistant Commissioner for Patents
Washington, D.C. 20231**

37 CFR 1.97(b)

1. ☒ The Information Disclosure Statement submitted herewith is being filed within three months of the filing of a national application other than a continued prosecution application under 37 CFR 1.53(d); within three months of the date of entry of the national stage as set forth in 37 CFR 1.491 in an international application; before the mailing of a first Office Action on the merits, or before the mailing of a first Office Action after the filing of a request for continued examination under 37 CFR 1.114.

37 CFR 1.97(c)

2. ☐ The Information Disclosure Statement submitted herewith is being filed after the period specified in 37 CFR 1.97(b), provided that the Information Disclosure Statement is filed before the mailing date of a Final Action under 37 CFR 1.113, a Notice of Allowance under 37 CFR 1.311, or an Action that otherwise closes prosecution in the application, and is accompanied by one of:
- ☐ the statement specified in 37 CFR 1.97(e);
- OR**
- ☐ the fee set forth in 37 CFR 1.17(p).

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Computer aided ligand-based and receptor-based drug utilizing molecular shape

Payment of Fee

(Only complete if Applicant elects to pay the fee set forth in 37 CFR 1.17(p))

- ☐ A check in the amount of _____ is attached.
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- ☐ Charge the amount of _____
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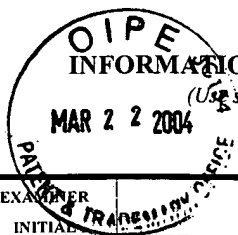
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Dated: March 18, 2003

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CERTIFICATE OF MAILING BY FIRST CLASS MAIL (37 CFR 1.8)			Docket No.	
Applicant(s):			30/1183US	
Serial No. 10/635,280	Filing Date 08/06/03	Examiner TBA	Group Art Unit TBA	
Invention: Computer aided ligand-based and receptor-based and receptor-based drug design utilizing molecular shape				
<p>I hereby certify that this <u>Initial Disclosure Citation, Transmittal of IDS, cited references and ack. p/c</u> (Identify type of correspondence)</p> <p>is being deposited with the United States Postal Service as first class mail in an envelope addressed to: The Commissioner of Patents and Trademarks, Washington, D.C. 20231-0001 on <u>March 18, 2004</u> (Date)</p> <p><u>Geralyn Spacher</u> (Typed or Printed Name of Person Mailing Correspondence)</p> <p><u>Geralyn Spacher</u> (Signature of Person Mailing Correspondence)</p>				
<p>Note: Each paper must have its own certificate of mailing.</p>				



INFORMATION DISCLOSURE CITATION (Use several sheets if necessary)	Docket Number (Optional) 30/1183US	Application Number 10/635,280
	Applicant(s) Randy J. Zauhar	
	Filing Date 08/06/03	Group Art Unit TBD

*EXAMINER INITIALS		OTHER DOCUMENTS (Including Author, Title, Date, Pertinent Pages, Etc.)
A		Klebe, G. Recent developments in structure-based drug design. J. Mol. Med. 2000, 78, 269-281.
B		Connolly, M. L. Analytical Molecular Surface Calculation. J. Appl. Crystallogr. 1983, 16, 548-558.
C		Chen, Z.; Li, Y.; Chen, E.; Hall, D.L.; Darke, P.L.; Culberson, C.; Shafer, J. A.; Kuo, L.C. Crystal structure at 1.9 Å resolution of human immunodeficiency virus (HIV) II protease complexed with L-735,524, an orally bioavailable inhibitor of the HIV proteases, J. Biol. Chem. 1994, 269, 26344.
D		Willett, P.; Barnard, J. M.; Downs, G. M. Chemical Similarity Searching. J. Chem. Inf. Comput. Sci. 1998, 38, 983-996.
E		Hahn, M. Three-Dimensional Shape-Based Searching of Conformationally Flexible Compounds, J. Chem. Inf. Comput. Sci. 1997, 37, 80-86.
F		Raymond J. W.; Willett, P. Maximum common subgraph isomorphism algorithms for the matching of chemical structures. J. Comput.-Aided Mol. Des. 2002, 16, 521-533.
G		Thorner, D. A.; Willett, P.; Wright, P.M.; Taylor, R. Similarity searching in files of three-dimensional chemical structures: representation and searching of molecular electrostatic potentials using field-graphs. J. Comput.-Aided Mol. Des. 1997, 11, 163-174.
H		Polanski, J.; Walczak, B. The comparative molecular surface analysis (COMSA): a novel tool for molecular design. Comput.Chem. 2000, 24, 615-625.
I		Hull, R. D.; Singh, S.B.; Nachbar, R.B.; Sheridan, R.P.; Kearsley, S.K.; Fluder, E.M. Latent semantic structure indexing (LaSSI) for defining chemical similarity. J. Med. Chem. 2001, 44, 1177-1184.
J		van Drie, J. H. 'Shrink-wrap' surfaces: A new method for incorporation shape into pharmacophoric 3D database searching. J. Chem. Inf. Comput. Sci. 1997, 37, 38.
K		Lawrence, M.C.; Colman, P.M. Shape complementarity at protein/protein interfaces. J. Mol. Biol. 1993, 234, 946-950.
L		Putta, S.; Lemmen, C.; Beroza, P.; Greene, J. A novel shape-feature based approach to virtual library screening. J. Chem. Inf. Comput. Sci. 2002, 42, 1230-1240.

EXAMINER	DATE CONSIDERED
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*EXAMINER: Initial if citation considered, whether or not citation is in conformance with MPEP Section 609; Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.

INFORMATION DISCLOSURE CITATION*(Use several sheets if necessary)*

Docket Number (Optional)

30/1183US

Application Number

10/635,280

Applicant(s)

Randy J. Zauhar

Filing Date

08/06/03

Group Art Unit

TBD

*EXAMINER
INITIAL**OTHER DOCUMENTS** *(Including Author, Title, Date, Pertinent Pages, Etc.)*

M

Cramer, R. D.; Patterson, D.E.; Bunce, J. D. Recent advances in comparative molecular field analysis (CoMFA). Prog. Clin. Biol. Res. 1989, 291, 161-165.

N

Cramer, R.D. Topomer CoMFA: a design methodology for rapid lead optimization. J. Med. Chem. 2003, 46, 374-388.

O

Gasteiger, J.; Marsili, M. Iterative partial equalization of orbital electronegativity-Rapid access to atomic charges. Tetrahedron 1980, 36, 3219-3288.

P

Ewing, T. J.; Makino, S.; Skillman, A. G.; Kuntz, I. D. DOCK 4.0: search strategies for automated molecular docking of flexible molecule databases. J. Comput.-Aided Mol. Des. 2001, 15, 411-428.

Q

Miller, M. D.; Kearsley, S. K.; Underwood, D. J.; Sheridan, R. P. FLOG: a system to select 'quasi-flexible' ligands complementary to a receptor of known three-dimensional structure. J. Comput.-Aided Mol. Des. 1994, 8, 153-174.

R

Jones, G; Willett, P; Glen, R. C.; Leach, A. R.; Taylor, R. Development and validation of a genetic algorithm for flexible docking. J. Mol. Biol. 1997, 267, 727-748.

S

Sitkoff, D.; Sharp, K. A.; Honig, B. Accurate Calculation of Hydration Free Energies Using Macroscopic Solvent Models. J. Phys. Chem. 1994, 98, 1978-1988.

T

Zauhar, R. J. SMART: a solvent-accessible triangulated surface generator for molecular graphics and boundary element applications. J. Comput.-Aided Mol. Des. 1995, 9, 149-159.

U

Richards, F. M. Areas, Volumes, Packing and Protein Structure. Annu. Rev. Biophys. Bioeng. 1977, 6, 151-176

V

Kuntz, I. D.; Blaney, J. M.; Oatley, S. J.; Langridge, R.; Ferrin, T.E. A geometric approach to macromolecule-ligand interactions. J. Mol. Biol. 1982, 161, 269-288.

W

Xue, L.; Barorath, J. Molecular descriptors in chemoinformatics, computational chemistry, and virtual screening. Comb. Chem. High Throughput Screen 2000, 3,363-372

X

Waszkowycz, B. Structure-based approaches to drug design and virtual screening. Curr. Opin. Drug Discov. Devel. 2002, 407-413.

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		Filing Date 08/06/03		Group Art Unit TBD	
*EXAMINER INITIAL		OTHER DOCUMENTS <i>(Including Author, Title, Date, Pertinent Pages, Etc.)</i>			
Y		Zehnacker, M.T.; Brennan, R.H.; Milne, G. W. A.; Miller, J.A. ; Hammel, M. J. The NCI Drug Information System 6. System Maintenance. J. Chem. Inf. Comput. Sci 1986, 26, 193-197.			
EXAMINER		DATE CONSIDERED			
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